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Exponential decay of eigenfunctions of Brown–Ravenhall operators

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Abstract
We prove the exponential decay of eigenfunctions of reductions of Brown–Ravenhall operators to arbitrary irreducible representations of rotation–reflection and permutation symmetry groups under the assumption that the corresponding eigenvalues are below the essential spectrum.

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1. Introduction

The Brown–Ravenhall operator can be considered as the (multiparticle) Dirac operator projected to the positive spectral subspace of free particles. This operator was introduced in [1] as a Hamiltonian of quantum electrodynamics (QED) correct to the second order in the fine structure constant (see also [2]). The higher order corrections predicted by QED should thus be treated as perturbations. The Brown–Ravenhall model turns out to be a good candidate for this approach, as the recent rigorous results show. Indeed, it is bounded below even in the many-particle case for physically relevant nuclear charges [3–5], and the structure of its spectrum resembles that of the Schrödinger operator—the essential spectrum forms a semiaxis [6–9], possibly with some eigenvalues below ionization thresholds [6, 9]. This is in a remarkable contrast to the many-particle Coulomb–Dirac operator which has an essential spectrum on the whole real axis and no eigenvalues, but is sometimes used as a formal unperturbed Hamiltonian in some QED calculations.

Having in mind the intention to consider the Brown–Ravenhall operator as an unperturbed intermediate model, it is very useful to have information on the rate of spatial decay of its eigenfunctions. In this paper, we prove that for systems of particles with electric charges of the same sign (we consider the potential energy of interactions with nuclei as an external field) the eigenfunctions decay exponentially, provided the corresponding eigenvalues are below the essential spectrum. This will also be proved for restrictions of the operator on subspaces of wavefunctions with certain rotation–reflection symmetries.

There are numerous results concerning the exponential decay of eigenfunctions of multiparticle Schrödinger operators, including anisotropic estimates and lower bounds. A very detailed analysis of the non-isotropic exponential decay of eigenfunctions of Schrödinger operators in terms of a metric in configuration space is presented in [10]. It is proved in [11] that the upper bound of [10] is exact at least for the ground state. A very simple proof of the exponential decay, based on the approach of [10], can be found in [12], lemma 6.2.

As for relativistic operators, the exponential decay of eigenfunctions is proved for one-particle Chandrasekhar operators [13, 14] and some projected multiparticle Dirac operators [15]. For one-particle Brown–Ravenhall atomic Hamiltonians, the exponential decay of eigenfunctions was first obtained in [16] for coupling constants of the Coulomb potential not exceeding $\frac{1}{2}$. In the recent preprint [17], the exponential decay of bigger rate is shown to hold pointwise for all one-electron atoms with subcritical or critical coupling constants.

This paper is organized as follows. In section 2, we introduce the Brown–Ravenhall model together with some auxiliary constructions and formulate the main result in theorem 2.3. Then in section 3 we discuss the relevant properties of the interaction potentials. The proof of theorem 2.3 is presented in section 4, with the proofs of technical lemmata postponed until sections 6–8. In section 5, we prepare these proofs recalling two useful theorems which give sufficient conditions for the boundedness of integral operators. The appendix contains a couple of properties of modified Bessel functions for reference.

2. The model and the main result

In the Hilbert space $L_2(\mathbb{R}^3, \mathbb{C}^4)$, the Dirac operator describing a particle of mass $m > 0$ is given by

$$D_m = -\mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta m,$$

where $\boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 Dirac matrices [18]. The form domain of D_m is the Sobolev space $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is $(-\infty, -m] \cup [m, +\infty)$. Let Λ_m be the orthogonal projector onto the positive spectral subspace of D_m:

$$\Lambda_m := \frac{1}{2} + \frac{-\mathrm{i}\boldsymbol{\alpha}\cdot\nabla + \beta m}{2\sqrt{-\Delta + m^2}}.$$

We consider a finite system of N particles with positive masses m_n, $n = 1, \ldots, N$. To simplify the notation we write D_n and Λ_n for D_{m_n} and Λ_{m_n}, and also for their tensor products with the identity operators in $L_2(\mathbb{R}^3, \mathbb{C}^4)$, e.g.

$$\bigotimes_{j=1}^{n-1} I \otimes D_{m_n} \otimes \bigotimes_{k=n+1}^{N} I \qquad \text{and} \qquad \bigotimes_{j=1}^{n-1} I \otimes \Lambda_{m_n} \otimes \bigotimes_{k=n+1}^{N} I,$$

respectively.

Let $\mathfrak{H}_N := \bigotimes_{n=1}^{N} \Lambda_n L_2(\mathbb{R}^3, \mathbb{C}^4)$ be the Hilbert space with the inner product induced by that on $\bigotimes_{n=1}^{N} L_2(\mathbb{R}^3, \mathbb{C}^4) \cong L_2(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$. In this space, the N-particle Brown–Ravenhall operator is formally defined by

$$\mathcal{H}_N = \Lambda^N \left(\sum_{n=1}^{N} (D_n + V_n) + \sum_{n<j}^{N} U_{nj} \right) \Lambda^N, \tag{2.1}$$

with

$$\Lambda^N := \prod_{n=1}^{N} \Lambda_n = \bigotimes_{n=1}^{N} \Lambda_n.$$

Here, the indices n and j indicate the particle on whose coordinates the corresponding operator acts.

In (2.1) V_n and U_{nj} are the operators of multiplication by the potential energy of interactions of the particles of the system with an external field and between themselves, respectively. In most applications to atomic and molecular physics, Brown–Ravenhall operators are considered in the Born–Oppenheimer approximation. Then V_n is the potential energy of the nth particle in the electrostatic field of static nuclei

$$V_n(\mathbf{x}_n) := e_n \sum_{k=1}^{K} \frac{z_k}{|\mathbf{x}_n - \mathbf{r}_k|}, \tag{2.2}$$

where e_n is the electric charge of the particle, and z_k and $\mathbf{r}_k$ are the charges and positions of the nuclei. The interaction between the particles is given by the Coulomb potential energy

$$U_{nj}(\mathbf{x}_n, \mathbf{x}_j) := \frac{e_n e_j}{|\mathbf{x}_n - \mathbf{x}_j|}. \tag{2.3}$$

We will assume that all the particles of the system have the same sign of electric charges e_n, $n = 1, \ldots, N$, but otherwise they might be different, as happens to *exotic atoms*, where some electrons are replaced with muons or even hadrons. The spin of each particle is assumed to be equal to 1/2, as always with Dirac and Brown–Ravenhall operators. This implies that the particles of the system are fermions. According to the Pauli principle, if some of the particles are identical, the wavefunction of the system should be antisymmetric under their permutations. This means that the operator (2.1) should be restricted to the subspace of $\mathfrak{H}_N$ consisting of functions which transform according to a certain irreducible representation E of a subgroup Π of the symmetric group $\mathcal{S}_N$ generated by transpositions of identical particles. Let P^E be the orthogonal projector in $\mathfrak{H}_N$ onto the space of such functions. We will denote the restriction of $\mathcal{H}_N$ on $\mathfrak{H}^E := P^E\mathfrak{H}$ by $\mathcal{H}_N^E$.

We will assume that the subcriticality condition

$$\min_{n,k} e_n z_k > -2(2/\pi + \pi/2)^{-1} \tag{2.4}$$

holds. According to [4], $\mathcal{H}_N$ (and thus $\mathcal{H}_N^E$) is bounded below even if we replace the strict inequality in (2.4) by a non-strict. Violation of such a non-strict inequality usually leads to the lack of boundedness below, as shown in [3] for the case of single nucleus. As far as $\mathcal{H}_N$ (or any of its restrictions) is bounded below, it can be defined via the corresponding quadratic form.

It is convenient to reduce $\mathcal{H}_N^E$ using the rotation–reflection symmetries of the system. Let γ be an orthogonal transform in $\mathbb{R}^3$: the rotation around the axis directed along a unit vector $\mathbf{n}_\gamma$ through an angle φ_γ, possibly combined with the reflection $\mathbf{x} \mapsto -\mathbf{x}$. The corresponding unitary operator O_γ acts on the functions $\psi \in \mathfrak{H}_N$ as (see [18], chapter 2)

$$(O_\gamma\psi)(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{n=1}^{N} \mathrm{e}^{-\mathrm{i}\varphi_\gamma \mathbf{n}_\gamma \cdot \mathbf{S}_n} \psi(\gamma^{-1}\mathbf{x}_1, \ldots, \gamma^{-1}\mathbf{x}_N).$$

Here $\mathbf{S}_n = -\frac{i}{4}\boldsymbol{\alpha}_n \wedge \boldsymbol{\alpha}_n$ is the spin operator acting on the spinor coordinates of the nth particle. The compact group of orthogonal transformations γ such that O_γ commutes with V_n and U_{nj} for all $n,\ j = 1, \ldots, N$ (and thus with $\mathcal{H}_N^E$) is denoted by Γ. Further, we decompose $\mathfrak{H}_N^E$ into the orthogonal sum

$$\mathfrak{H}_N^E = \bigoplus_{T \in \mathrm{Irr}\,\Gamma} \mathfrak{H}_N^{T,E}, \tag{2.5}$$

where $\mathfrak{H}_N^{T,E}$ consists of functions form $\mathfrak{H}_N^E$ which transforms under O_γ according to some irreducible representation T of Γ. The decomposition (2.5) reduces $\mathcal{H}_N^E$. We denote the self-adjoint restrictions of $\mathcal{H}_N^E$ to $\mathfrak{H}_N^{T,E}$ by $\mathcal{H}_N^{T,E}$. The spectrum of $\mathcal{H}_N^E$ is the union of the spectra of $\mathfrak{H}_N^{T,E}$, $T \in \operatorname{Irr}\Gamma$.

Together with the whole system of N particles we will consider its decompositions into two clusters. Such decompositions play an important role in the characterization of the essential spectrum of the operators $\mathfrak{H}_N^{T,E}$. Let $Z = (Z_1, Z_2)$ be a decomposition of the index set $I := \{1, \ldots, N\}$ into two disjoint subsets:

$$I = Z_1 \cup Z_2, \qquad Z_1 \cap Z_2 = \varnothing.$$

Let

$$\widetilde{\mathcal{H}}_{Z,1} := \sum_{n\in Z_1} (D_n + V_n) + \sum_{\substack{n,j\in Z_1\\ n<j}} U_{nj}, \tag{2.6}$$

$$\widetilde{\mathcal{H}}_{Z,2} := \sum_{n\in Z_2} D_n + \sum_{\substack{n,j\in Z_2\\ n<j}} U_{nj}. \tag{2.7}$$

We introduce the operators corresponding to noninteracting clusters, with the second cluster transferred far away from the sources of the external field:

$$\mathcal{H}_{Z,j} := \Lambda_{Z,j}\widetilde{\mathcal{H}}_{Z,j}\Lambda_{Z,j}, \qquad \text{in} \quad \mathfrak{H}_{Z,j} := \bigotimes_{n\in Z_j} \Lambda_n L_2(\mathbb{R}^3, \mathbb{C}^4), \qquad j = 1, 2, \tag{2.8}$$

where

$$\Lambda_{Z,j} := \prod_{n\in Z_j} \Lambda_n = \bigotimes_{n\in Z_j} \Lambda_n.$$

For a given cluster decomposition $Z = (Z_1, Z_2)$ we denote by P^{E_j} and P^{T_j} the projectors onto the irreducible representations E_j and T_j of the restrictions of Π and Γ, respectively, on the cluster of particles indexed by Z_j, $j = 1, 2$.

Given representations T_j and E_j, projector $P^{T_j}P^{E_j} = P^{E_j}P^{T_j}$ reduces $\mathcal{H}_{Z,j}$. We denote the reduced operators in

$$\mathfrak{H}_{Z,j}^{T_j,E_j} := P^{T_j}P^{E_j}\mathfrak{H}_{Z,j}$$

by $\mathcal{H}_{Z,j}^{T_j,E_j}$ and define

$$\varkappa_j(Z, T_j, E_j) := \inf \operatorname{Spec}\mathcal{H}_{Z,j}^{T_j,E_j}. \tag{2.9}$$

We write $(T_1, E_1; T_2, E_2) \underset{Z}{\prec} (T, E)$ if the corresponding term cannot be omitted on the rhs of

$$\mathfrak{H}_N^{T,E} \subset \bigoplus_{\substack{(T_1,E_1)\\(T_2,E_2)}} \left(\mathfrak{H}_{Z,1}^{T_1,E_1} \otimes \mathfrak{H}_{Z,2}^{T_2,E_2}\right)$$

without violation of the inclusion. For $Z_2 \neq \varnothing$ let

$$\varkappa(Z, T, E) := \begin{cases} \inf\limits_{(T_1,E_1;T_2,E_2)\underset{Z}{\prec}(T,E)} \{\varkappa_1(Z, T_1, E_1) + \varkappa_2(Z, T_2, E_2)\}, & Z_1 \neq \varnothing,\\ \varkappa_2(Z, T, E), & Z_1 = \varnothing, \end{cases} \tag{2.10}$$

and

$$\varkappa(T, E) := \min\{\varkappa(Z, T, E) : Z = (Z_1, Z_2),\ Z_2 \neq \varnothing\}. \tag{2.11}$$

We are now ready to characterize the essential spectrum of $\mathcal{H}_N^{T,E}$ in terms of cluster decompositions.

Theorem 2.1 (Morozov [9], theorem 6)**.** *For $N \in \mathbb{N}$ let T be some irreducible representation of Γ, and E some irreducible representation of Π, such that $P^T P^E \neq 0$. The essential spectrum of $\mathcal{H}_N^{T,E}$ is $[\varkappa(T, E), \infty)$.*

Thus, the bottom of the essential spectrum is equal to the minimal energy which the system can have if some of the particles are transferred far away form other particles and sources of the external field. We will omit the proof of the following simple proposition based on the positivity of the interaction potentials (2.3).

Proposition 2.2. *It is enough to take the minimum in (2.11) over Z with $Z_2 = \{n\}$, $n = 1, \dots, N$. Moreover, for such Z, $\varkappa_2(Z, \cdot, \cdot)$ in (2.10) is equal to m_n, the mass of the particle in the second cluster.*

As shown in [6], the Brown–Ravenhall operators $\mathcal{H}_N^{T,E}$ can have eigenvalues below the essential spectrum. Note that in view of the decomposition (2.5) these eigenvalues can be embedded in the essential spectrum of $\mathfrak{H}_N^E$.

Our main result is the following theorem.

Theorem 2.3. *For $N \in \mathbb{N}$ let T be some irreducible representation of Γ, and E some irreducible representation of Π, such that $P^T P^E \neq 0$. Let ϕ be an eigenfunction of $\mathcal{H}_N^{T,E}$ corresponding to an eigenvalue λ below the essential spectrum, i.e.*

$$\mathcal{H}_N^{T,E}\phi = \lambda\phi, \qquad \lambda < \varkappa(T, E).$$

Then there exists $S > 0$ independent of λ and ϕ such that for

$$s := \min\left\{\frac{1}{2\sqrt{N}}, (\varkappa(T, E) - \lambda)S\right\}$$

it holds

$$\int_{\mathbb{R}^{3N}} \mathrm{e}^{2s|\mathbf{X}|}|\phi(\mathbf{X})|^2 \, \mathrm{d}\mathbf{X} < \infty. \tag{2.12}$$

Note that for λ close to the bottom of the essential spectrum s behaves linearly in $(\varkappa(T, E) - \lambda)$. However, for Schrödinger [10], Dirac [19], Chandrasekhar [14] and one-particle Brown–Ravenhall operators [17] s can be chosen to be proportional to the square root of this distance. This suggests a conjecture that for the multiparticle operators we are considering the actual rate of decay might have this property as well. But the proof of such a conjecture is yet obscure even in view of [17], since that result is obtained by comparison to the decay rate of the eigenfunctions of the Dirac operator, which are nonexistent in the multiparticle case.

3. Some properties of the model

In this section, we single out some simple properties of the multiparticle Brown–Ravenhall operators introduced in the previous section. The reason for doing so is twofold. First, it will allow the reader to see which properties are required in each step of the subsequent proof of the exponential decay. Second, this will allow us to reformulate the main result without referring to the explicit form of the potentials (2.2) and (2.3), thus making future generalizations easier.

We need a bit of notation. Let $\{\Omega_j\}_{j=1}^N$ be a collection of uniformly C^1-regular domains in $\mathbb{R}^3$ with bounded boundaries. For $n = 1, \ldots, N$, $s \in \mathbb{R}$, and $\Omega = \mathop{\times}\limits_{j=1}^{N} \Omega_j$ we introduce the anisotropic Sobolev spaces

$$H_n^s(\Omega, \mathbb{C}^{4^N}) := \left(\bigotimes_{j=1}^{n-1} L_2(\Omega_j, \mathbb{C}^4)\right) \otimes H^s(\Omega_n, \mathbb{C}^4) \otimes \left(\bigotimes_{j=n+1}^{N} L_2(\Omega_j, \mathbb{C}^4)\right).$$

Property 3.1. *For any $R > 0$ there exists a finite $C_R \geqslant 0$ such that*

$$\sum_{n=1}^{N} \left(\int_{|\mathbf{x}|\leqslant R} |V_n(\mathbf{x})|^2\, \mathrm{d}\mathbf{x}\right)^{1/2} + \sum_{n<j}^{N} \left(\int_{|\mathbf{x}|\leqslant R} |U_{nj}(\mathbf{x})|^2\, \mathrm{d}\mathbf{x}\right)^{1/2} \leqslant C_R.$$

In other words, the interaction potentials are locally square integrable.

Property 3.2. *The external field potentials decay at infinity in the L_∞-norm:*

$$\lim_{R\to\infty} \operatorname*{ess\,sup}_{|\mathbf{x}|>R} |V_n(\mathbf{x})| = 0, \qquad n = 1, \ldots, N. \tag{3.1}$$

Property 3.3. *For any $\varepsilon > 0$ there exists $R > 0$ big enough such that for all $n < j = 1, \ldots, N$*

$$\|U_{nj}\psi\|_{L_2(\mathbb{R}^{3N}\cap\{|\mathbf{x}_n-\mathbf{x}_j|>R\})} \leqslant \varepsilon \min_{k=n,j} \|\psi\|_{H_k^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}, \qquad \text{for all} \quad \psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}).$$

Proof. This follows from the weaker property

$$\lim_{R\to\infty} \operatorname*{ess\,sup}_{|\mathbf{x}_n-\mathbf{x}_j|>R} |U_{nj}(\mathbf{x})| = 0, \qquad n, j = 1, \ldots, N$$

of the potentials (2.3). □

Property 3.4. *The interparticle interaction potentials are nonnegative:*

$$U_{nj} \geqslant 0, \qquad \text{for all} \quad n < j = 1, \ldots, N. \tag{3.2}$$

This follows from the assumption that all the particles of the system have electric charges of the same sign.

Property 3.5. *There exists $C > 0$ such that for any $n = 1, \ldots, N$*

$$|\langle V_n\varphi, \psi\rangle| \leqslant C\|\varphi\|_{H_n^{1/2}}\|\psi\|_{H_n^{1/2}}, \qquad \text{for any} \quad \varphi, \psi \in H_n^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}), \tag{3.3}$$

and for any $n < j = 1, \ldots, N$

$$|\langle U_{nj}\varphi, \psi\rangle| \leqslant C\|\varphi\|_{H^{1/2}}\|\psi\|_{H^{1/2}}, \qquad \text{for any} \quad \varphi, \psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}). \tag{3.4}$$

Proof. Inequalities (3.3) and (3.4) follow from Kato's inequality (see [20] and [21], theorem 2.9a). □

Property 3.6. *There exists $C > 0$ such that for any $n = 1, \ldots, N$ and any $\psi \in H^1(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$*

$$\|U_{nj}\psi\| \leqslant C \min_{k=n,j} \|\psi\|_{H_k^1(\mathbb{R}^{3N},\mathbb{C}^{4^N})}. \tag{3.5}$$

It is not surprising to have the minimum on the rhs of (3.5), since U_{nj} only depends on the difference $\mathbf{x}_n - \mathbf{x}_j$. Note that (3.5) can be applied even if ψ is only known to belong either to $H_n^1(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ or to $H_j^1(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$.

Proof. Inequality (3.5) follows from Hardy's inequality (see e.g. [22], p. 55) and the properties of symmetric-decreasing rearrangements (see e.g. [23], lemma 7.17 and relation (3.3.4)). □

Property 3.7. *There exist $C_1 > 0$ and $C_2 \in \mathbb{R}$ such that for any cluster decomposition Z*

$$\langle \mathcal{H}_{Z,j}\psi, \psi\rangle \geqslant C_1 \left\langle \sum_{n\in Z_j} D_n\psi, \psi \right\rangle - C_2\|\psi\|^2,$$

$$\text{for any} \quad \psi \in \bigotimes_{n\in Z_j} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4), \qquad j = 1, 2. \tag{3.6}$$

Proof. This is where we need the subcriticality condition (2.4). According to the result of [4], inequality (2.4) implies (3.6) if $N = 1$. For $N > 1$ it is enough to use property 3.4 to estimate $\mathcal{H}_{Z,j}$ from below by a direct sum of one-particle operators. □

Remark 3.8. By properties 3.5 and 3.7, the quadratic forms of operators (2.8) (and, in particular, $\mathcal{H}_N$) are bounded below and closed on $\bigotimes_{n\in Z_j} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Thus, these operators are well defined in the form sense, and so are their restrictions to invariant subspaces.

Remark 3.9. Suppose that the potentials (2.2) and (2.3) are replaced by operators of multiplication by some measurable Hermitian matrix-valued functions such that V_n are the operators of multiplication of spinor coordinates of the nth particle by 4×4 matrix-valued functions $V_n(\mathbf{x}_n)$, $n = 1, \ldots, N$, and U_{nj} are the operators of multiplication of spinor coordinates of nth and jth particles by 16×16 matrix-valued functions $U_{nj}(\mathbf{x}_n - \mathbf{x}_j)$, $n < j = 1, \ldots, N$. Then the statements of theorems 2.1 and 2.3 remain valid, provided properties 3.1–3.7 hold. Indeed, properties 3.1–3.7 imply assumptions 1–5 of [9], which form the hypothesis of theorem 6 of [9]. And in the proof of theorem 2.3, we will not need the explicit expressions (2.2) and (2.3), but only the properties listed in this section.

4. Proof of theorem 2.3

Some constants in the proof can depend on the masses of the particles. Since we only deal with a finite number of particles with positive masses, such dependence will not be indicated explicitly.

Lemma 4.1. *Suppose that for some $a > 0$*

$$\int_{\mathbb{R}^{3N}} e^{2a|\mathbf{x}_n|}|\phi(\mathbf{X})|^2\, d\mathbf{X} < \infty, \qquad n = 1, \ldots, N. \tag{4.1}$$

Then (2.12) holds with $s = N^{-1/2}a$.

Proof.

$$e^{2s|\mathbf{X}|} \leqslant e^{2\sqrt{N}s \max_{n=1,\ldots,N}|\mathbf{x}_n|} \leqslant \sum_{n=1}^{N} e^{2\sqrt{N}s|\mathbf{x}_n|} = \sum_{n=1}^{N} e^{2a|\mathbf{x}_n|}.$$

Thus, (4.1) implies (2.12) after summation in n. □

It remains to prove that (4.1) holds with some suitable $a > 0$. Without loss of generality we will consider the case $n = 1$.

Let $\rho \in C^2([0,\infty),[0,\infty))$ be given by

$$\rho(z) := \begin{cases} z^2 - \dfrac{z^3}{3}, & z \in [0,1), \\ z - \dfrac{1}{3}, & z \in [1,\infty). \end{cases} \tag{4.2}$$

For $\epsilon > 0$ let

$$f(\mathbf{X}) := f(\mathbf{x}_1) := \frac{\rho(|\mathbf{x}_1|)}{1+\epsilon\rho(|\mathbf{x}_1|)}. \tag{4.3}$$

Note that for any $\epsilon > 0$

$$\|\nabla f\|_{L_\infty} < 1. \tag{4.4}$$

Since $\phi \in L_2(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$, for $n = 1$ (4.1) is equivalent to

$$\|e^{af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})} \leqslant C \tag{4.5}$$

with C being independent of ϵ. Note that for any $\epsilon > 0$ the function e^{af} is twice differentiable with bounded derivatives. Hence multiplication by e^{af} is a bounded operator in the Sobolev spaces $H^s(\mathbb{R}^3, \mathbb{C}^4)$ with $s \in [0, 2]$.

The following two lemmata will be important in the subsequent proof.

Lemma 4.2. *For any $a_0 \in [0,1)$ there exists $C(a_0) > 0$ such that for any $a \in [0, a_0]$ and $\psi \in L_2(\mathbb{R}^3, \mathbb{C}^4)$*

$$\|[\Lambda_1, e^{af}]\psi\|_{H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a\|e^{af}\psi\| \tag{4.6}$$

and

$$\|e^{-af}[\Lambda_1, e^{af}]\psi\|_{H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a\|\psi\|. \tag{4.7}$$

Lemma 4.2 is proved in section 6. Some analogous estimates with L_2-norms instead of H^1-norms can be found in [16].

Corollary 4.3. *For any $a_0 \in [0,1)$ there exists $C(a_0) > 0$ such that for any $a \in [0, a_0]$ and $\psi \in L_2(\mathbb{R}^3, \mathbb{C}^4)$*

$$\|e^{-af}\Lambda_1 e^{af}\psi\| \leqslant C(a_0)\|\psi\|. \tag{4.8}$$

Proof.

$$e^{-af}\Lambda_1 e^{af} = \Lambda_1 + e^{-af}[\Lambda_1, e^{af}],$$

and (4.7) implies (4.8). □

Lemma 4.4. *Let B_R be the ball of radius $R > 0$ in $\mathbb{R}^3$ centred at the origin. For any $a \in [0, 1/2)$ there exist $C(R) > 0$ and $C(a,R) > 0$ such that for any $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$*

$$\|\Lambda_1\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} \leqslant C(R)\|\psi\|_{H^{1/2}(B_{3R},\mathbb{C}^4)} + C(a,R)\|e^{-2af}\psi\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}. \tag{4.9}$$

We prove lemma 4.4 in section 7.

In order to be able to apply lemma 4.4 we will only consider $a \in [0, 1/2)$. We can thus fix $a_0 \in [1/2, 1)$ and no longer trace the dependence of the constants in lemma 4.2 and corollary 4.3 on this parameter.

Let us fix a cluster decomposition

$$Z_0 := (\{2,\ldots,N\},\{1\}). \tag{4.10}$$

Then

$$\Lambda_1 e^{af}\phi = P^T P^E \Lambda_1 e^{af}\phi = \sum_{(T_1,E_1;T_2,1)\underset{Z_0}{\prec}(T,E)} (P^{T_1}P^{E_1} \otimes P^{T_2})\Lambda_1 e^{af}\phi. \tag{4.11}$$

The eigenfunction ϕ belongs to the form domain of $\mathcal{H}_N^{T,E}$, which is

$$P^T P^E \bigotimes_{n=1}^{N} \Lambda_n H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \subset H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N}).$$

Hence by (4.11), (2.9), (2.10) and (2.11)

$$\begin{aligned}
&\langle \Lambda_1 e^{af}\phi, (\mathcal{H}_{Z_0,1} + \mathcal{H}_{Z_0,2})\Lambda_1 e^{af}\phi\rangle \\
&\quad \geqslant \left\langle \Lambda_1 e^{af}\phi, \sum_{(T_1,E_1;T_2,1)\underset{Z_0}{\prec}(T,E)} (\varkappa_1(Z_0,T_1,E_1) + \varkappa_2(Z_0,T_2,1))(P^{T_1}P^{E_1} \otimes P^{T_2})\Lambda_1 e^{af}\phi \right\rangle \\
&\quad \geqslant \varkappa(T,E)\|\Lambda_1 e^{af}\phi\|^2.
\end{aligned} \tag{4.12}$$

Let us introduce

$$Q_1 := \varkappa(T,E)\langle e^{af}\phi, [e^{af}, \Lambda_1]\phi\rangle, \tag{4.13}$$

$$Q_2 := \left\langle \Lambda_1 e^{af}\phi, \left(\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\right)[\Lambda_1, e^{af}]\phi \right\rangle, \tag{4.14}$$

$$Q_3 := \langle \Lambda_1 e^{af}\phi, [D_1, e^{af}]\phi\rangle, \tag{4.15}$$

$$Q_4 := -\left\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, \left(V_1 + \sum_{j=2}^{N} U_{1j}\right)\phi \right\rangle. \tag{4.16}$$

Then by (4.12) (recall the definitions (2.6)–(2.8) and (2.1))

$$\begin{aligned}
\varkappa(T,E)\|e^{af}\phi\|^2 &= \langle \Lambda_1 e^{af}\phi, \varkappa(T,E)\Lambda_1 e^{af}\phi\rangle + Q_1 \\
&\leqslant \langle \Lambda_1 e^{af}\phi, (\mathcal{H}_{Z_0,1} + \mathcal{H}_{Z_0,2})\Lambda_1 e^{af}\phi\rangle + Q_1 \\
&= \left\langle \Lambda_1 e^{af}\phi, \left(\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\right) e^{af}\phi \right\rangle + Q_1 + Q_2 \\
&= \left\langle \Lambda_1 e^{af}\phi, e^{af}\left(\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj} + D_1\right)\phi \right\rangle + \sum_{l=1}^{3} Q_l \\
&= \langle \Lambda_1 e^{af}\phi, e^{af}\mathcal{H}_N^{T,E}\phi\rangle + \sum_{l=1}^{4} Q_l = \lambda\|\Lambda_1 e^{af}\phi\|^2 + \sum_{l=1}^{4} Q_l \\
&\leqslant \lambda\|e^{af}\phi\|^2 + \sum_{l=1}^{4} Q_l.
\end{aligned} \tag{4.17}$$

Thus

$$(\varkappa(T,E) - \lambda)\|e^{af}\phi\|^2 \leqslant \sum_{l=1}^{4} Q_l, \tag{4.18}$$

and it remains to estimate $Q_1, \ldots, Q_4$. This will be done in the following four lemmata.

Lemma 4.5. *There exists a positive constant C_1 such that*

$$|Q_1| \leqslant C_1 a \|e^{af}\phi\|^2. \tag{4.19}$$

Proof. By (4.13) and lemma 4.2 we have

$$|Q_1| \leqslant |\varkappa(T,E)| \|e^{af}\phi\| \|[e^{af}, \Lambda_1]\phi\| \leqslant Ca|\varkappa(T,E)| \|e^{af}\phi\|^2. \qquad \square$$

Lemma 4.6. *There exists a positive constant C_2 such that*

$$|Q_2| \leqslant C_2 a \|e^{af}\phi\|^2. \tag{4.20}$$

Proof. Since Λ_1 commutes with $\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj}$, $\phi = \Lambda_1\phi$ and $\Lambda_1[\Lambda_1, e^{af}]\Lambda_1 = 0$, we have

$$\left\langle \Lambda_1 e^{af}\phi, \left(\sum_{n=2}^{N}(D_n + V_n) + \sum_{1<n<j}^{N} U_{nj}\right)[\Lambda_1, e^{af}]\phi \right\rangle = 0. \tag{4.21}$$

According to lemma 4.2

$$|\langle \Lambda_1 e^{af}\phi, D_1[\Lambda_1, e^{af}]\phi\rangle| \leqslant \|\Lambda_1 e^{af}\phi\| \| |D_1| [\Lambda_1, e^{af}]\phi\| \leqslant Ca\|e^{af}\phi\|^2.$$

By (4.14) and (4.21) this implies (4.20). $\square$

Lemma 4.7. *There exists a positive constant C_3 such that*

$$|Q_3| \leqslant C_3 a \|e^{af}\phi\|^2. \tag{4.22}$$

Proof. We have $[D_1, e^{af}] = [-i\alpha\cdot\nabla, e^{af}] = -i\alpha\cdot(\nabla e^{af}) = -i\alpha\cdot a(\nabla f)e^{af}$. Now (4.22) follows from (4.15) and (4.4). $\square$

Lemma 4.8. *There exist $C_4 > 0$ and $C_0(a) > 0$ such that*

$$Q_4 \leqslant C_4 a \|e^{af}\phi\|^2 + C_0(a)\|\phi\|^2_{H^{1/2}}. \tag{4.23}$$

We give a proof of lemma 4.8 in section 8.

Substituting the estimates (4.19), (4.20), (4.22) and (4.23) into (4.18), we conclude that

$$\left(\varkappa(T,E) - \lambda - a\sum_{l=1}^{4} C_l\right) \|e^{af}\phi\|^2 \leqslant C_0(a)\|\phi\|^2_{H^{1/2}}. \tag{4.24}$$

Now if

$$a < \min\left\{\frac{1}{2}, \left(\sum_{l=1}^{4} C_l\right)^{-1} (\varkappa(T,E) - \lambda)\right\},$$

then the expression in brackets on the lhs of (4.24) is positive, and (4.24) implies (4.5) with a finite C independent of ϵ. Theorem 2.3 is proved.

5. Boundedness of integral operators

In this section, we collect some auxiliary material for the subsequent proofs of lemmata 4.2, 4.4 and 4.8. In order to be able to obtain the information on the boundedness of (singular) integral operators, we will need the following two theorems.

Theorem 5.1. *(Stein [24], chapter 2, section 3.2) Let $K : \mathbb{R}^n \to \mathbb{C}$ be a measurable function such that for some $B > 0$*

$$|K(\mathbf{x})| \leqslant B|\mathbf{x}|^{-n}, \qquad |\nabla K(\mathbf{x})| \leqslant B|\mathbf{x}|^{-n-1}, \qquad \text{for almost every} \quad \mathbf{x} \in \mathbb{R}^n$$

and

$$\int_{R_1<|\mathbf{x}|<R_2} K(\mathbf{x})\mathrm{d}^n\mathbf{x} = 0, \qquad \text{for all} \quad 0 < R_1 < R_2 < \infty.$$

For $g \in L_p(\mathbb{R}^n)$, $1 < p < \infty$, let

$$A_\varepsilon(g)(\mathbf{x}) := \int_{|\mathbf{x}-\mathbf{y}|\geqslant\varepsilon} K(\mathbf{x}-\mathbf{y})g(\mathbf{y})\mathrm{d}^n\mathbf{y}, \qquad \varepsilon > 0.$$

Then

$$\|A_\varepsilon(g)\|_p \leqslant B_p\|g\|_p \tag{5.1}$$

with B_p being independent of g and ε.

Remark 5.2. Inequality (5.1) shows that the operator $A := \lim_{\varepsilon\to+0} A_\varepsilon$ exists as a bounded operator in $L_p(\mathbb{R}^n)$ and its norm satisfies $\|A\|_p \leqslant B_p$.

The second theorem is known as Schur's test.

Theorem 5.3. *Let (Ω_1, μ_1) and (Ω_2, μ_2) be two spaces with measures. Let $A(\cdot,\cdot)$ be a measurable (matrix) function on $\Omega_1 \times \Omega_2$ satisfying*

$$M_1 := \sup_{\mathbf{y}\in\Omega_2} \int_{\Omega_1} |A(\mathbf{x},\mathbf{y})|\mathrm{d}\mu_1(\mathbf{x}) < \infty, \qquad M_2 := \sup_{\mathbf{x}\in\Omega_1} \int_{\Omega_2} |A(\mathbf{x},\mathbf{y})|\mathrm{d}\mu_2(\mathbf{y}) < \infty.$$

Then the integral operator

$$(A\psi)(\mathbf{x}) := \int_{\Omega_2} A(\mathbf{x},\mathbf{y})\psi(\mathbf{y})\mathrm{d}\mu_2(\mathbf{y})$$

is bounded from $L_2(\Omega_2)$ to $L_2(\Omega_1)$ and $\|A\| \leqslant \sqrt{M_1M_2}$.

We will only use theorem 5.3 in the case $\Omega_1 = \Omega_2 = \mathbb{R}^3$ with Lebesgue measure.

Note that in the case of convolution (i.e. for $A(\mathbf{x},\mathbf{y}) = A(\mathbf{x}-\mathbf{y})$, $\Omega_1 = \Omega_2 = \mathbb{R}^d$), theorem 5.3 reduces to Young's inequality for convolution with L_1-function (see e.g. [25]).

For a 4×4 measurable matrix function A on $\mathbb{R}^3\times\mathbb{R}^3$ we define the corresponding integral operator by

$$(Ag)(\mathbf{x}) := \lim_{\varepsilon\to+0} \int_{|\mathbf{x}-\mathbf{y}|>\varepsilon} A(\mathbf{x},\mathbf{y})g(\mathbf{y})\mathrm{d}\mathbf{y}, \qquad g \in C_0^1(\mathbb{R}^3,\mathbb{C}^4). \tag{5.2}$$

We will only work with such A for which (5.2) is well defined and extends to a bounded operator in $L_2(\mathbb{R}^3,\mathbb{C}^4)$ either by theorem 5.1 (in which case $A(\mathbf{x},\mathbf{y})$ has to depend only on $(\mathbf{x}-\mathbf{y})$) or by theorem 5.3.

In particular, according to the definition given above and appendix B of [6], the integral kernel of $(\Lambda_m - 1/2)$ is

$$\mathcal{K}(\mathbf{x},\mathbf{y}) = \mathcal{K}(\mathbf{x}-\mathbf{y}) := \frac{\mathrm{i}m}{2\pi^2}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}K_1(m|\mathbf{x}-\mathbf{y}|) + \frac{m^2}{4\pi^2}\left(\beta\frac{K_1(m|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|} + \frac{\mathrm{i}\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}K_0(m|\mathbf{x}-\mathbf{y}|)\right). \tag{5.3}$$

The boundedness follows from theorem 5.1 and (A.2).

Note that the function (5.3) rapidly decays together with its derivatives if $|\mathbf{x}-\mathbf{y}|$ becomes big. Namely, if for $r > 0$ we define

$$G(r) := \sup_{|\mathbf{x}-\mathbf{y}|>r}|\mathcal{K}(\mathbf{x},\mathbf{y})| + \sup_{|\mathbf{x}-\mathbf{y}|>r}|\nabla_{\mathbf{x}}\mathcal{K}(\mathbf{x},\mathbf{y})|, \tag{5.4}$$

then by (A.2) and the first asymptotic in (A.1), for any $R > 0$ there exists $C(R) > 0$ such that

$$G(r) \leqslant C(R)r^{-3/2}\mathrm{e}^{-r}, \qquad \text{for all} \quad r \geqslant R. \tag{5.5}$$

We will also use the following elementary lemma (lemma 10 of [9]).

Lemma 5.4. *For any $d, k \in \mathbb{N}$ there exists $C > 0$ such that for any bounded differentiable function χ on $\mathbb{R}^d$ with bounded gradient and $u \in H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)$*

$$\|\chi u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} \leqslant C(\|\chi\|_{L_\infty(\mathbb{R}^d)} + \|\nabla\chi\|_{L_\infty(\mathbb{R}^d)})\|u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)}.$$

6. Proof of lemma 4.2

To prove (4.6) it is enough to show that $[\Lambda_1, \mathrm{e}^{af}]\mathrm{e}^{-af}$ is a bounded operator from $L_2(\mathbb{R}^3,\mathbb{C}^4)$ to $H^1(\mathbb{R}^3,\mathbb{C}^4)$ satisfying

$$\|[\Lambda_1, \mathrm{e}^{af}]\mathrm{e}^{-af}\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C(a_0)a, \qquad a \in [0, 1). \tag{6.1}$$

The integral kernel of $[\Lambda_1, \mathrm{e}^{af}]\mathrm{e}^{-af} = \left[(\Lambda_1 - 1/2), \mathrm{e}^{af}\right]\mathrm{e}^{-af}$ is given by (see (5.3))

$$([\Lambda_1, \mathrm{e}^{af}]\mathrm{e}^{-af})(\mathbf{x},\mathbf{y}) = \mathcal{K}(\mathbf{x},\mathbf{y})(1 - \mathrm{e}^{a(f(\mathbf{x})-f(\mathbf{y}))}), \tag{6.2}$$

and its gradient in $\mathbf{x}$ is

$$(\nabla[\Lambda_1, \mathrm{e}^{af}]\mathrm{e}^{-af})(\mathbf{x},\mathbf{y}) = (\nabla_{\mathbf{x}}\mathcal{K})(\mathbf{x},\mathbf{y})(1 - \mathrm{e}^{a(f(\mathbf{x})-f(\mathbf{y}))}) + a\mathcal{K}(\mathbf{x},\mathbf{y})(1 - \mathrm{e}^{a(f(\mathbf{x})-f(\mathbf{y}))})(\nabla f)(\mathbf{x}) - a\mathcal{K}(\mathbf{x},\mathbf{y})(\nabla f)(\mathbf{x}). \tag{6.3}$$

We rewrite

$$1 - \mathrm{e}^{a(f(\mathbf{x})-f(\mathbf{y}))} = -a(\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + R_1(\mathbf{x},\mathbf{y}) + R_2(\mathbf{x},\mathbf{y}), \tag{6.4}$$

where

$$R_1(\mathbf{x},\mathbf{y}) := 1 + a(f(\mathbf{x}) - f(\mathbf{y})) - \mathrm{e}^{a(f(\mathbf{x})-f(\mathbf{y}))}$$

and

$$R_2(\mathbf{x},\mathbf{y}) := a((\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + f(\mathbf{y}) - f(\mathbf{x})).$$

Since

$$|\mathrm{e}^z - 1 - z| \leqslant (\mathrm{e}-2)z^2 \qquad \text{for} \quad |z| \leqslant 1,$$

by (4.4) we have

$$|R_1(\mathbf{x},\mathbf{y})| \leqslant (\mathrm{e}-2)a^2(f(\mathbf{x}) - f(\mathbf{y}))^2 \leqslant (\mathrm{e}-2)a^2|\mathbf{x}-\mathbf{y}|^2, \quad \text{for} \quad |\mathbf{x}-\mathbf{y}| \leqslant a^{-\frac{1}{2}}. \tag{6.5}$$

On the other hand, since $a < a_0 < 1$, for $|\mathbf{x}-\mathbf{y}| > a^{-\frac{1}{2}}$ the functions

$$|\mathcal{K}(\mathbf{x},\mathbf{y})R_1(\mathbf{x},\mathbf{y})| \qquad \text{and} \qquad |\nabla_{\mathbf{x}}\mathcal{K}(\mathbf{x},\mathbf{y})R_1(\mathbf{x},\mathbf{y})|$$

are integrable in $\mathbf{x}$ or $\mathbf{y}$ with the integrals bounded by $C(a_0)a$, as follows from (5.4), (5.5) and (4.4). Since $f \in C^2(\mathbb{R}^3)$, by the Taylor formula we have

$$f(\mathbf{x}) - f(\mathbf{y}) = (\nabla f)(\mathbf{y})\cdot(\mathbf{x}-\mathbf{y}) + \langle(\mathcal{D}f)(\xi\mathbf{x}+(1-\xi)\mathbf{y})(\mathbf{x}-\mathbf{y}), (\mathbf{x}-\mathbf{y})\rangle_{\mathbb{R}^3},$$

where $\mathcal{D}f$ is the Hessian matrix (i.e. the matrix of the second partial derivatives of f) and $\xi \in [0,1]$. Hence

$$|R_2(\mathbf{x},\mathbf{y})| = a|\langle(\mathcal{D}f)(\xi\mathbf{x}+(1-\xi)\mathbf{y})(\mathbf{x}-\mathbf{y}), (\mathbf{x}-\mathbf{y})\rangle_{\mathbb{R}^3}| \leqslant a\|\mathcal{D}f\|_{L_\infty}|\mathbf{x}-\mathbf{y}|^2, \tag{6.6}$$

where $\|\mathcal{D}f\|_{L_\infty}$ is bounded uniformly in ϵ by (4.3) and (4.2). Substituting (6.4) into (6.2) and (6.3), and using the estimates (6.5)–(6.6) we obtain (6.1) by theorems 5.1 and 5.3. This completes the proof of (4.6).

The proof of (4.7) is completely analogous since the integral kernel of

$$\mathrm{e}^{-af}[\Lambda_1, \mathrm{e}^{af}] = \mathrm{e}^{-af}[(\Lambda_1 - 1/2), \mathrm{e}^{af}]$$

is

$$\mathcal{K}(\mathbf{x},\mathbf{y})(\mathrm{e}^{a(f(\mathbf{y})-f(\mathbf{x}))} - 1)$$

(compare with (6.2)).

7. Proof of lemma 4.4

Let $\eta \in C^\infty(\mathbb{R}^3, [0,1])$ with

$$\eta(\mathbf{x}) \equiv \begin{cases} 0, & \mathbf{x} \in B_{2R}, \\ 1, & \mathbf{x} \in \mathbb{R}^3 \setminus B_{3R}. \end{cases}$$

Since Λ_1 is a bounded operator in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, by lemma 5.4 we have

$$\begin{aligned}\|\Lambda_1\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} &\leqslant \|\Lambda_1(1-\eta)\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} + \|\Lambda_1\eta\psi\|_{H^{1/2}(B_R,\mathbb{C}^4)} \\ &\leqslant C(R)\|\psi\|_{H^{1/2}(B_{3R},\mathbb{C}^4)} + \|\Lambda_1\eta\psi\|_{H^1(B_R,\mathbb{C}^4)}.\end{aligned} \tag{7.1}$$

By (5.4) we can estimate the second term on the rhs of (7.1) as

$$\begin{aligned}
&\|\Lambda_1\eta\psi\|^2_{H^1(B_R,\mathbb{C}^4)} \\
&= \int_{B_R}\left(\left|\int_{|\mathbf{y}|>2R} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2 + \left|\int_{|\mathbf{y}|>2R}\nabla_{\mathbf{x}}K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2\right)\mathrm{d}\mathbf{x} \\
&\leqslant \frac{4}{3}\pi R^3 \sup_{\mathbf{x}\in B_R}\left(\left|\int_{|\mathbf{y}|>2R} K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2 + \left|\int_{|\mathbf{y}|>2R}\nabla_{\mathbf{x}}K(\mathbf{x},\mathbf{y})\eta(\mathbf{y})\psi(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2\right) \\
&\leqslant \frac{4}{3}\pi R^3\left(\int_{|\mathbf{y}|>2R}\left(\sup_{\mathbf{x}\in B_R}|K(\mathbf{x},\mathbf{y})| + \sup_{\mathbf{x}\in B_R}|\nabla_{\mathbf{x}}K(\mathbf{x},\mathbf{y})|\right)|\psi(\mathbf{y})|\mathrm{d}\mathbf{y}\right)^2 \\
&\leqslant \frac{4}{3}\pi R^3\left(\int_{|\mathbf{y}|>2R} G(|\mathbf{y}|-R)|\psi(\mathbf{y})|\mathrm{d}\mathbf{y}\right)^2 \\
&\leqslant \frac{4}{3}\pi R^3\left(\int_{|\mathbf{y}|>2R} G^{1-2a}(|\mathbf{y}|-R)\mathrm{d}\mathbf{y}\right)\left(\int_{|\mathbf{y}|>2R} G^{1+2a}(|\mathbf{y}|-R)|\psi(\mathbf{y})|^2\mathrm{d}\mathbf{y}\right).
\end{aligned}$$

Since $a < 1/2$ and $f(\mathbf{x}) \leqslant |\mathbf{x}|$, we conclude from (5.5) that there exists $C(a, R)$ such that

$$\|\Lambda_1\eta\psi\|_{H^1(B_R,\mathbb{C}^4)} \leqslant C(a,R)\|\mathrm{e}^{-2af}\psi\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)},$$

and (4.9) follows by (7.1).

8. Proof of lemma 4.8

For $j = 2, \ldots, N$ we have

$$\langle \Lambda_1 e^{af} \Lambda_1 e^{af} \phi, U_{1j}\phi \rangle = \langle U_{1j} e^{af}\phi, e^{af}\phi \rangle + \langle U_{1j} e^{-af}[\Lambda_1, e^{af}]\Lambda_1 e^{af}\phi, e^{af}\phi\rangle + \langle U_{1j}[\Lambda_1, e^{af}]\phi, e^{af}\phi\rangle. \tag{8.1}$$

The first term on the rhs of (8.1) is nonnegative by (3.2). Applying (3.5), lemma 4.2 and Schwarz inequality we can estimate the last two terms by $Ca\|e^{af}\phi\|^2$. Hence by (4.16)

$$Q_4 \leqslant Ca\|e^{af}\phi\|^2 + |\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle| \tag{8.2}$$

and it remains to estimate the last term on the rhs of (8.2).

Let $\chi_1 \in C^\infty(\mathbb{R}^3, [0, 1])$ be a function supported in $\mathbb{R}^3\backslash B_1$ such that it is equal to 1 on $\mathbb{R}^3\backslash B_2$. For $R > 1$ let

$$\chi_R(\mathbf{X}) := \chi_R(\mathbf{x}_1) := \chi_1(\mathbf{x}_1/R).$$

We have

$$|\langle \Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle| \leqslant |\langle e^{-af}\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, \chi_R V_1 e^{af}\phi\rangle| + |\langle (1-\chi_R)\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle|. \tag{8.3}$$

By corollary 4.3,

$$\|e^{-af}\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\| \leqslant C\|e^{af}\phi\|. \tag{8.4}$$

Since χ_R is supported outside B_R, by (3.1) we have

$$\|\chi_R V_1 e^{af}\phi\| \leqslant \varepsilon(R)\|e^{af}\phi\|, \qquad \varepsilon(R) \underset{R\to\infty}{\longrightarrow} 0. \tag{8.5}$$

According to (3.3),

$$|\langle (1-\chi_R)\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle| \leqslant C\|(1-\chi_R)\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}}\|\phi\|_{H_1^{1/2}}. \tag{8.6}$$

Since $(1-\chi_R)$ is a smooth function supported in $\{|\mathbf{x}_1| \leqslant 2R\}$, by lemmata 5.4 and 4.4 we have

$$\begin{aligned}\|(1-\chi_R)\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}} &\leqslant C(R)\|\Lambda_1 e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{2R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})}\\ &\leqslant C(R)\|e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} + C(a,R)\|e^{-af}\Lambda_1 e^{af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}.\end{aligned} \tag{8.7}$$

By corollary 4.3 the second term on the rhs of (8.7) can be estimated by $C(a,R)\|\phi\|$. Applying lemma 4.4 to the first term we obtain

$$\begin{aligned}&C(R)\|e^{af}\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})}\\ &\quad\leqslant C(a,R)\|\Lambda_1 e^{af}\phi\|_{H_1^{1/2}(B_{6R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})}\\ &\quad\leqslant C(a,R)\|e^{af}\phi\|_{H_1^{1/2}(B_{18R}\times\mathbb{R}^{3N-3},\mathbb{C}^{4^N})} + C(a,R)\|e^{-af}\phi\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\\ &\quad\leqslant C(a,R)\|\phi\|_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}.\end{aligned} \tag{8.8}$$

Thus by (8.6)–(8.8)

$$|\langle (1-\chi_R)\Lambda_1 e^{af}\Lambda_1 e^{af}\phi, V_1\phi\rangle| \leqslant C(a,R)\|\phi\|^2_{H^{1/2}}. \tag{8.9}$$

Estimating the rhs of (8.3) according to (8.4), (8.5) and (8.9) and substituting the result into (8.2) we obtain

$$Q_4 \leqslant Ca\|e^{af}\phi\|^2 + C\varepsilon(R)\|e^{af}\phi\|^2 + C(a,R)\|\phi\|^2_{H^{1/2}}.$$

Choosing R so that $\varepsilon(R) \leqslant a$ we arrive at (4.23). Lemma 4.8 is proved.

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Appendix A. Some properties of modified Bessel functions

The modified Bessel (McDonald) functions are related to the Hankel functions by the formula

$$K_\nu(z) = \frac{\pi}{2} \mathrm{e}^{\mathrm{i}\pi(\nu+1)/2} H_\nu^{(1)}(\mathrm{i}z).$$

These functions are positive and decreasing for $z \in (0, \infty)$. Their asymptotics are (see [26] 8.446, 8.447.3, 8.451.6)

$$K_\nu(z) = \sqrt{\frac{\pi}{2z}} \mathrm{e}^{-z} \left(1 + \mathrm{O}\left(\frac{1}{z}\right)\right), \qquad z \to +\infty;$$

$$K_0(z) = -\log z(1 + \mathrm{o}(1)), \qquad K_1(z) = \frac{1}{z}(1 + \mathrm{o}(1)), \qquad z \to +0. \tag{A.1}$$

The derivatives of these functions are (see [26] 8.486.12, 8.486.18)

$$K_0'(z) = -K_1(z), \qquad K_1'(z) = -K_0(z) - \frac{1}{z} K_1(z), \qquad z \in (0, \infty). \tag{A.2}$$

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